

Effects of broadening on BCS theory in the presence of Van Hove singularities

D. R. Penn

Electron Physics Group, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

Marvin L. Cohen

Department of Physics, University of California, Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, California 94720

(Received 2 December 1991)

There have been recent suggestions that high- T_c superconductivity can be understood in terms of conventional BCS theory if there is a logarithmic Van Hove singularity in the electron density of states near the Fermi energy as suggested by band theory. We consider the effects of broadening of the singularity on theories of this type. The broadening may be caused by inhomogeneities arising from doping or structural defects, electron inelastic scattering, and three-dimensional dispersion.

I. INTRODUCTION

There is at present no established theory of high- T_c superconductivity in the oxides. It has recently been suggested that a simple modification of the usual BCS theory might be able to account for high values of T_c as well as small values of the isotope coefficient α for the superconducting oxides. The physical basis for this modification is found in the density-of-states peaks suggested by band-structure calculations. If the Fermi energy lies near a singularity in the density of states then the usual BCS-type expressions for T_c and α are modified. This possibility was stressed by Labbe and Bok¹ and by Friedel² for the high- T_c oxides. Very recently Tsuei *et al.*³ (to be referred to as TNCP) showed that this approach is consistent with the anomalous behavior of α as a function of doping x in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ as measured by Crawford *et al.*⁴

Labbe and Bok as well as Friedel derived an expression for T_c for the case where the Fermi energy lies at the logarithmic singularity, and they pointed out that the isotope coefficient is greatly reduced from its BCS value of 0.5. Following earlier work by Tsuei,⁵ TNCP generalized the theory by not constraining the Fermi energy to lie at the singularity and carried out a calculation of T_c and α as a function of the energy separation between the Fermi energy and the singularity. A similar situation was considered⁶ earlier for both weak and strong coupling for planar structure in the density of states.

The logarithmic singularity upon which these theories are based is a two-dimensional Van Hove singularity. It has been pointed out by previous workers² that, in principle, this singularity can be removed by a broadening of the electronic states or by the presence of three-dimensional effects. In this paper we describe a quantitative study of the consequences of introducing broadening into the density of states. Three sources of broadening will be considered: (1) inhomogeneities, (2) three-dimensional effects, and (3) inelastic electron scattering. The first two sources are represented by a constant ener-

gy broadening and the third by a broadening proportional to temperature.

We will show that for materials such as Y-Ba-Cu-O the presence of a logarithmic singularity in the density of states (as treated within the model of TNCP) is not sufficient to explain the very small isotope coefficient even in the absence of broadening. For La-Sr-Cu-O with an intermediate value of the isotope coefficient, $\alpha=0.14$, it is found that the effects of broadening depend on whether this broadening is constant or proportional to temperature, and on the energy separation between the Fermi energy and the singularity. For values of the broadening consistent with band-structure calculations, the theory fails to explain the measured properties.

II. THEORY AND DISCUSSION

The broadening due to disorder caused by doping and structural defects is modeled by a parameter Γ that is taken to be constant. The logarithmic singularity in the density of states in TNCP is replaced by

$$N(E) = N_0 \ln \left[\frac{\epsilon_F}{\sqrt{(\epsilon_F - \epsilon)^2 + \Gamma^2}} \right], \quad (1)$$

where N_0 is independent of energy. In the case $\Gamma=0$, $N(E)$ is the density of states assumed in the previous studies.

Three-dimensional band dispersion can also be characterized by a constant broadening. In two dimensions the surfaces of constant energy are shown in Fig. 1 in the (k_x, k_y) plane as has been discussed by Friedel.² The location of the singularity is at an energy corresponding to the square Fermi surface. If there were no dispersion in the k_z direction, this picture would remain valid. In the presence of dispersion the two-dimensional Van Hove singularity is replaced by three-dimensional critical points. For example, if dispersion in the z direction is represented by an additional term in the energy of the form $t_\perp \cos(k_z a)$, then there are saddle points at $k_z=0$

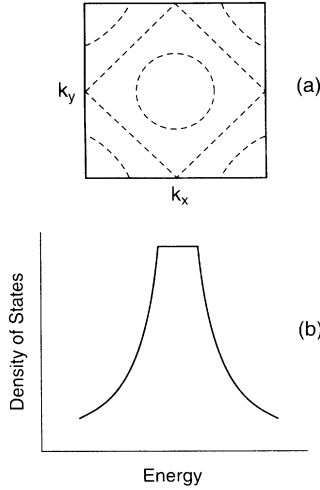


FIG. 1. (a) Surfaces of constant energy in two dimensions for the model band structure discussed in Ref. 2. A logarithmic singularity is located at an energy corresponding to the equal Fermi surfaces. (b) Form of the three-dimensional density of states that obtains if a term of the form $t_1 \sin(k_x a)$ is added to the two-dimensional band structure.

and $k_z = \pm \pi/a$ and the logarithmic singularity is replaced by the structure shown in Fig. 1(b). In this case, we approximate the density of states shown in Fig. 1(b) by Eq. (1) with $\Gamma = t_1/2$ if ϵ_F lies in the center of the peak.

Finally, broadening of the electron states due to the electron-phonon interaction has been suggested⁷ to be important in limiting the value of T_c in the A15 compounds. The form of the broadening caused by the electron-phonon interaction is given by

$$\Gamma_{\text{ep}} = 2\pi\lambda_{\text{T}} k_B T, \quad (2)$$

where λ_{T} is often taken to be the superconducting coupling parameter λ . Although Eq. (2) is usually assumed to be valid for temperatures T greater than the Debye temperature, the observed resistivity in the high-temperature superconductors is linear for $T \geq T_c$ and thus for this case we assume the presence of a temperature-dependent broadening of this form,

$$\Gamma = \beta T, \quad (3)$$

in Eq. (1). We find that the temperature dependence of the broadening leads to a very different expression for α than for the case of a constant broadening. The quantity β can be estimated from the resistivity, however, in view of the uncertainties in this procedure and the large value of Γ that arises from band dispersion, no estimate of β is made here.

The BCS expression for T_c is

$$\frac{2}{V} = \int_{\epsilon_F - \hbar\omega_D}^{\epsilon_F + \hbar\omega_D} \frac{d\epsilon}{\epsilon - \epsilon_F} \tanh \left[\frac{\epsilon - \epsilon_F}{2k_B T_c} \right] N(\epsilon), \quad (4)$$

where V is the strength of the attractive interaction, $\hbar\omega_D$ is the Debye energy, and the density of states is taken to be

$$N(\epsilon) = N_0 \ln \left[\frac{E_F}{\sqrt{(\epsilon - \epsilon_F - \delta)^2 + \Gamma^2}} \right], \quad (5)$$

where δ is the energy separation of the singularity from the Fermi energy and Γ is the broadening. In the case that Γ is zero, Eq. (5) reduces to the density of states in TNCP. The isotope coefficient α is given by

$$\alpha = - \frac{M}{T_c} \frac{\partial T_c}{\partial M}, \quad (6)$$

and may be evaluated from Eq. (4) using $\hbar\omega_D \propto M^{-1/2}$ where M is the ionic mass.

In order to evaluate T_c and α from Eqs. (4) and (6) in the case of $\Gamma = 0$ considered in TNCP, the following approximation was introduced:

$$\begin{aligned} \tanh x &= x, \quad x \leq 1, \\ \tanh x &= 1, \quad x > 1. \end{aligned} \quad (7)$$

In the limit $\delta = 0$, TNCP obtained

$$T_c = 1.36 T_F \exp(-\{2/N_0 V - 1 + [\ln(\epsilon_F/\hbar\omega_D)]^2\}^{1/2}) \quad (8a)$$

and

$$\alpha = \frac{1}{2} [\ln(T_F/\hbar\omega_D)/\ln(1.36 T_F/T_c)]. \quad (8b)$$

A result similar to Eq. (8a) is given in Refs. 1 and 2. Equation (8) shows that T_c can be enhanced and α reduced by the logarithmic singularity in the density of states. In the pre-exponential factor of Eq. (8a), T_F replaces $\hbar\omega_D$ in the usual BCS result and the exponential factor replaces $1/N_0 V$ with a resultant enhancement in T_c . Similarly, the BCS result for α is $\alpha = \frac{1}{2}$, and it is clear from Eq. (8b) that α can be reduced below $\frac{1}{2}$. However, it is immediately apparent that Eq. (8b) for α cannot explain the very small isotope shift observed in Y-Ba-Cu-O. For example, using the parameters relevant for Y-Ba-Cu-O, $\hbar\omega_D = 754$ K, $T_F = 5800$ K, and $T_c = 92$ K from TNCP yields $\alpha = 0.23$, which is much larger than the observed value of 0.02.

In the general case, where $\delta \neq 0$ and $\Gamma \neq 0$, use of Eq. (7) in Eq. (4) yields an analytic expression for isotope shift (but not for T_c). The isotope shift as computed using Eqs. (4), (6), and (7) is denoted by α_0 or α_T for the cases Γ constant and $\Gamma \propto T$, respectively. The results are as follows:

$$\alpha_0 = A/(B + C), \quad (9a)$$

$$\alpha_T = A/(B - D - E), \quad (9b)$$

$$A = \frac{1}{2}(L_W^+ + L_W^-), \quad (9c)$$

$$B = D^+ L_T^+ + D^- L_T^- - 4, \quad (9d)$$

$$C = \left[\frac{\bar{\Gamma}}{\bar{T}_c} \right] \left[\tan^{-1} \left[\frac{T^+}{\bar{\Gamma}} \right] + \tan^{-1} \left[\frac{T^-}{\bar{\Gamma}} \right] \right], \quad (9e)$$

$$D = \left[1 + \left[\frac{\bar{\delta}}{\bar{\Gamma}} \right]^2 \right]^{-1} \left[4 \ln \left[\frac{\bar{\omega}_D}{2\bar{T}_c} \right] + L_T^+ + L_T^- - L_W^+ - L_W^- \right], \quad (9f)$$

$$E = 2 \left[\left[\frac{\bar{\Gamma}}{\bar{\delta}} \right] + \left[\frac{\bar{\delta}}{\bar{\Gamma}} \right] \right]^{-1} \times \left[\tan^{-1} \left[\frac{W^-}{\bar{\Gamma}} \right] - \tan^{-1} \left[\frac{W^+}{\bar{\Gamma}} \right] + \tan \left[\frac{T^+}{\bar{\Gamma}} \right] - \tan^{-1} \left[\frac{T^-}{\bar{\Gamma}} \right] \right], \quad (9g)$$

$$W^\pm = \bar{\omega}_D \pm \bar{\delta}, \quad (9h)$$

$$L_W^\pm = \ln[(W^\pm)^2 + \bar{\Gamma}^2], \quad (9i)$$

$$D^\pm = 1 \pm \bar{\delta}/2\bar{T}_c, \quad (9j)$$

$$L_T^\pm = \ln[(T^\pm)^2 + \bar{\Gamma}^2], \quad (9k)$$

$$T^\pm = 2\bar{T}_c \pm \bar{\delta}, \quad (9l)$$

$$\bar{\omega}_D = \frac{\omega_D}{\epsilon_F}, \quad \bar{\delta} = \frac{\delta}{\epsilon_F}, \quad \bar{T}_c = \frac{k_B T_c}{\epsilon_F}, \quad \bar{\Gamma} = \frac{\Gamma}{\epsilon_F}. \quad (9m)$$

In the case $\bar{\delta}=0$, Eq. (9) gives

$$\alpha_0 = \frac{1}{2} \ln(\bar{\omega}_D^2 + \bar{\Gamma}^2) / \{ \ln[(2\bar{T}_c)^2 + \bar{\Gamma}^2] - 2 + (\bar{\Gamma}/\bar{T}_c) \tan^{-1}(2\bar{T}_c/\bar{\Gamma}) \}, \quad (10a)$$

$$\alpha_T = \frac{1}{2} \ln(\bar{\omega}_D^2 + \bar{\Gamma}^2) / \{ \ln(\bar{\omega}_D^2 + \bar{\Gamma}^2) - 2 - 2 \ln(\bar{\omega}_D/2\bar{T}_c) \}. \quad (10b)$$

If $\bar{\Gamma}=0$, Eq. (9) yields

$$\alpha_0 = \alpha_T = \frac{1}{2} \ln(\bar{\omega}_D^2 - \bar{\delta}^2) / \{ (1 + \bar{\delta}/2\bar{T}_c) \ln(2\bar{T}_c + \bar{\delta}) + (1 - \bar{\delta}/2\bar{T}_c) \ln(2\bar{T}_c - \bar{\delta}) - 2 \}. \quad (11)$$

Equations (9), (10), and (11) give the result (8b) when $\bar{\Gamma}=\bar{\delta}=0$. The case $\bar{\Gamma}=0$ is that studied in TNCP. Equation (11) shows that the isotope coefficient is singular at $\bar{\delta}=\bar{\omega}_D$ (or $\delta=\hbar\omega_c$ in the notation of TNCP). This is not an artifact of the approximation given by Eq. (7) as will be seen below in Eq. (12c).

The effect of a finite broadening in the case of $\bar{\delta}=0$ is given by Eq. (10). It is seen that $\alpha_0 \neq \alpha_T$; the two expressions differ significantly with $\alpha_T < \alpha_0$. For example, if the broadening satisfies $2\bar{T}_c \ll \bar{\Gamma} \ll \bar{\omega}_D$, then $\alpha_0 = \frac{1}{2}(\ln \bar{\omega}_D)/\ln \bar{\Gamma}$ and $\alpha_T = \frac{1}{2}(\ln \bar{\omega}_D)/[\ln(2\bar{T}_c) - 1]$. From Eq. (10b), if $\bar{\Gamma} \ll \bar{\omega}_D$, α_T is equal to its value for the case of no broadening, $\bar{\Gamma}=0$. This is not true of α_0 , which increases rapidly with increasing $\bar{\Gamma}$. The behavior $\alpha_T < \alpha_0$ arises because α measures the change of T_c with

M . As M increases, T_c decreases, and this decrease determines α_0 . However, if $\bar{\Gamma}$ is proportional to T , then a decrease in T_c results in a decrease in the broadening, which implies an increase in $N(E)$ and consequently in T_c . These opposing effects result in $\alpha_T < \alpha_0$.

The expressions for T_c and α are now evaluated numerically from Eqs. (4)–(6) without the use of the approximation of Eq. (7). The isotope coefficients $\bar{\alpha}_0$ and $\bar{\alpha}_T$ are given by

$$\bar{\alpha}_0 = \bar{A}/I_1, \quad (12a)$$

$$\bar{\alpha}_T = \bar{A}/(I_1 - I_2), \quad (12b)$$

where

$$\bar{A} = \bar{T}_c \tanh(\bar{\omega}_c/2\bar{T}_c) \ln \{ [(\bar{\omega}_c - \bar{\delta})^2 + \bar{\Gamma}^2][(\bar{\omega}_c + \bar{\delta})^2 + \bar{\Gamma}^2] \}, \quad (12c)$$

$$I_1 = \int_0^{\bar{\omega}_c} d\xi \ln \{ [(\xi - \bar{\delta})^2 + \bar{\Gamma}^2][(\xi + \bar{\delta})^2 + \bar{\Gamma}^2] \} / [\cosh(\xi/2\bar{T}_c)]^2, \quad (12d)$$

$$I_2 = 4\bar{T}_c \bar{\Gamma}^2 \int_0^{\bar{\omega}_c} \frac{d\xi}{\xi} \tanh \left[\frac{\xi}{2\bar{T}_c} \right] \left[\frac{1}{(\xi - \bar{\delta})^2 + \bar{\Gamma}^2} + \frac{1}{(\xi + \bar{\delta})^2 + \bar{\Gamma}^2} \right]. \quad (12e)$$

where $\xi = \epsilon/\epsilon_F$.

Results for La-Sr-Cu-O using the parameters of TNCP, $\bar{\omega}_c=0.13$ and $\bar{T}_c=0.0069$ are shown in Figs. 2 and 3 as a function of $\bar{\Gamma}$ for fixed values of $\bar{\delta}$. The case $\bar{\Gamma}=0$ is the one considered in TNCP. Even in the case $\bar{\Gamma}=0$, the theory gives too large a result for α , $\bar{\alpha}_0=\bar{\alpha}_T=0.2$. This is in disagreement with TNCP, which reported a value of 0.14. We do find agreement with the numerical results for TNCP for values of $\bar{\delta} \gtrsim 0.4$. The presence of even moderate values of broadening is seen to increase $\bar{\alpha}_0$,

whereas $\bar{\alpha}_T$, the isotope shift that occurs if the broadening is proportional to temperature, remains fairly constant for the case $\bar{\delta}=0$. The value of V required to maintain the correct value of T_c increases with increasing broadening. Band calculations⁸ indicate values of $\bar{\Gamma}$ might easily be as large as 0.2; that is, $\Gamma=0.1$ eV, which would substantially change the results of TNCP and give an isotope coefficient of 0.33. For the case of $\bar{\delta}=0.065$, the isotope coefficient is 0.4 with no broadening, in agreement with TNCP. In this case, we find that $\bar{\alpha}_0$ remains

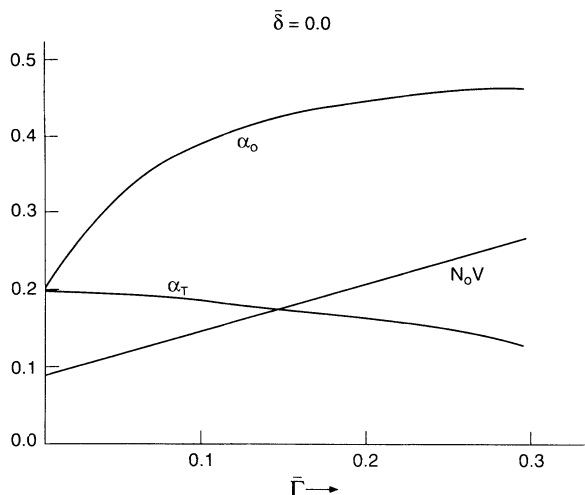


FIG. 2. Isotope coefficients α_0, α_T , and attractive electron interaction N_0V for La-Sr-Cu-O vs the reduced broadening parameter $\bar{\Gamma} = \Gamma/\varepsilon_F$ for the case $\bar{\delta} = \delta/\varepsilon_F = 0.0$. The isotope coefficients α_0, α_T correspond to the cases where $\bar{\Gamma}$ is independent of or proportional to temperature and δ is the energy difference between the Fermi energy and the position of the density-of-states singularity.

relatively constant with increasing broadening while $\bar{\alpha}_T$ shows a strong decrease.

III. SUMMARY

In summary, we have introduced broadening in theories that postulate a logarithmic singularity in the electronic density of states. This broadening is taken to be constant for the purpose of describing effects due to doping, inhomogeneities, and three-dimensional band dispersion. The broadening is assumed proportional to temperature in the case of inelastic electron scattering by phonons. Our goal was to give a more quantitative ac-

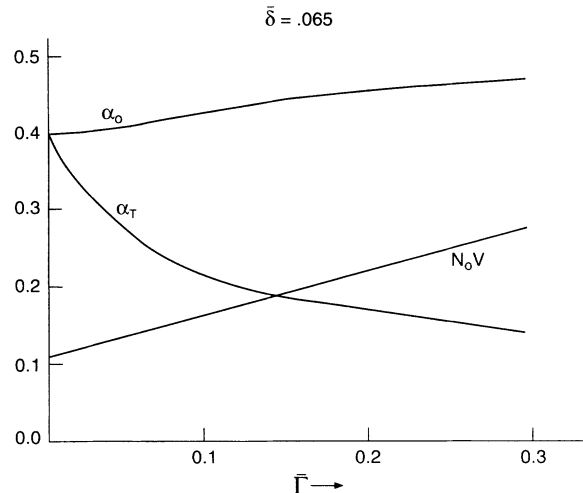


FIG. 3. Same as Fig. 2 but $\bar{\delta} = 0.065$.

count of the effects of broadening than was done by previous workers. The results are summarized in Figs. 2 and 3, where the effects on the isotope shift and the attractive electron-electron pairing interaction are shown. We conclude that the effects of broadening on these quantities can be substantial for values of the broadening suggested by band calculations, and such effects may present a serious obstacle to theories based on a logarithmic singularity in the electronic density of states.

ACKNOWLEDGMENTS

One of us (M.L.C.) acknowledges support for this work by National Science Foundation Grant No. DMR88-18404 and by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. He also acknowledges partial support from the J. S. Guggenheim Foundation.

- ¹J. Labbe and J. Bok, *Europhys. Lett.* **3**, 1225 (1987); J. Labbe, *Phys. Sci.* **T29**, 82 (1989); R. Combescot and J. Labbe, *Phys. Rev. B* **38**, 262 (1988).
- ²J. Friedel, *J. Phys.* **48**, 1787 (1987); *J. Phys. Condens. Matter.* **1**, 7757 (1989).
- ³C. C. Tsuei, D. M. Newns, C. C. Chi, and P. C. Pattnaik, *Phys. Rev. Lett.* **65** 2724 (1990).
- ⁴M. K. Crawford, M. N. Kunchur, W. E. Farneth, E. M.

- McCarron III, and S. J. Poon, *Phys. Rev. B* **41**, 282 (1990).
- ⁵C. C. Tsuei, *Physica A* **168**, 238 (1990).
- ⁶S. G. Lie and J. P. Carbotte, *Solid State Commun.* **34**, 599 (1980); E. Schachinger, M. G. Greenson, and J. P. Carbotte, *Phys. Rev. B* **42**, 406 (1990).
- ⁷K. M. Ho, M. L. Cohen, and W. E. Pickett, *Phys. Rev. Lett.* **41**, 815 (1978).
- ⁸W. E. Pickett (private communication).